Ground state energy of the low density Hubbard model. An upper bound.

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We derive an upper bound on the ground state energy of the three-dimensional (3D) repulsive Hubbard model on the cubic lattice agreeing in the low density limit with the known asymptotic expression of the ground state energy of the dilute Fermi gas in the continuum. As a corollary, we prove an old conjecture on the low density behavior of the 3D Hubbard model, i.e., that the total spin of the ground state vanishes as the density goes to zero.

I. INTRODUCTION

Recent developments in the theory of low density Bose and Fermi gases made it possible to verify old conjectures on the leading asymptotics for the ground state energy of dilute gases of bosons or fermions in the continuum, interacting with positive short range potentials. While the heuristing argument suggesting that the ground state energy of the 3D hard-core Bose gas is proportional to the scattering length a of the potential goes back to Lenz [Le], the first ideas in the direction of proving that Lenz's formula is correct in the low density limit are due to Dyson [D], who first established an asymptotically correct upper bound and a rigorous (but 14 times too small) lower bound for the hard core Bose gas in 3 dimensions. An asymptotically correct lower bound was proven much more recently by Lieb and Yngvason [LY]. Their work inspired much of the recent developments in the rigorous theory of low density quantum many body systems, see [LSSY] for a comprehensive review of the subject till 2005. In particular, a result that we would like to mention, strictly related to the problem studied in this paper, is the proof in [LSS] that the ground state energy per unit volume of the 3D Fermi gas in the continuum with short range repulsive interaction (and scattering length $a > 0$) is given, in the low density limit $\rho a^3 \to 0$, by:

$$e(\rho_\uparrow, \rho_\downarrow) = \frac{\hbar^2}{2m}\frac{3}{5}(6\pi^2)^{2/3}(\rho_\uparrow^{5/3} + \rho_\downarrow^{5/3}) + \frac{\hbar^2}{2m}8\pi a\rho_\uparrow\rho_\downarrow + o(a\rho^2) \tag{1.1}$$

where $\rho_{\uparrow,\downarrow}$ are the densities of spin up and spin down particles and m is their mass. Moreover $\rho = \rho_\uparrow + \rho_\downarrow$ and $o(a\rho^2)$ is a suitable function of the total density ρ and of the scattering length a vanishing faster than $a\rho^2$ in the limit $\rho a^3 \to 0$.

It is very natural to ask whether a formula similar to (1.1) is valid for a dilute Fermi gas with short range repulsive interaction on the lattice and, in particular, for the most popular model for correlated electrons in condensed matter physics: the Hubbard model. The Hubbard model is the simplest possible lattice model of interacting electrons displaying many "real world" features and in the last 40 years it has been subject of intense research efforts. Nonetheless, even its qualitative behavior in 2 or 3 dimensions is far from clear and there are very few rigorous results available in the literature. A survey of known results and open problems in the Hubbard model can be found in [Li] and in [T].

In the present paper we shall derive an upper bound for the ground state energy of the 3D repulsive Hubbard model on the cubic lattice with the same asymptotic behavior as (1.1). As a corollary we shall prove one of the open problems posed by Elliott Lieb in his review article on the Hubbard model (see [Li, Problem 3]). More precisely, we shall prove the following old conjecture on the low density behavior of the 3D Hubbard model.

Proposition. *Let $S_{max} = N_{tot}/2$ be the maximum spin a system of N_{tot} electrons can achieve and let S be the spin of the ground state of the 3D repulsive Hubbard model in a cubic*

box $\Lambda \subset \mathbb{Z}^3$ in presence of N_{tot} electrons (or the maximum such spin in case of degeneracy). Then

$$\lim_{\rho\to 0}\lim_{|\Lambda|\to\infty} S/S_{max} = 0\,, \tag{1.2}$$

where the thermodynamic limit is taken keeping the total density $\rho = N_{tot}/|\Lambda|$ fixed.

Remark. A sketch of the proof of this claim already appeared in [BLT]: in this note we provide all the details of the necessary computations as well as an explicit bound on the rate of convergence (see Corollary 1 below). Our strategy imitates the one in [LSS].

The paper is organized as follows. In the next two subsections we shall introduce the model, introduce the notion of scattering length and state the main results, i.e., the upper bound on the ground state energy and an explicit bound on the rate of convergence of S/S_{max} to 0 in (1.2). In Sec.II and in the two Appendices we shall give the proof.

A. The model

Given a cubic lattice Λ of lattice spacing r_0, the Hamiltonian of the Hubbard model on Λ for N spin-up particles and M spin-down particles can be written as:

$$H = -\Delta_X - \Delta_Y + U v_{XY} \tag{1.3}$$

where:
1) $X = (x_1, \dots, x_N)$ and $Y = (y_1, \dots, y_M)$ are the coordinates of the spin-up and spin-down particles, respectively;
2) $\Delta_X = \sum_{i=1}^N \Delta_{x_i}$, $\Delta_Y = \sum_{j=1}^M \Delta_{y_j}$ and $\Delta_x f(x) = r_0^{-2}\sum_{x':|x'-x|=r_0}(f(x') - f(x))$;
3) $v_{XY} = \sum_{i=1}^N\sum_{j=1}^M \delta_{x_i,y_j}$;
4) $U \geq 0$;
5) H acts on the space of functions antisymmetric in the X and in the Y coordinates separately and vanishing outside the box Λ (Dirichlet boundary conditions).

Remark. In this note we restrict for simplicity to the case of a nearest neighbor hopping and a delta interaction, however the analysis below can be generalized to cases with different hopping terms and different short range interactions (not necessarily zero - or finite - range).

We want to obtain an upper bound for the ground state energy that is asymptotically correct, at the lowest order, as $\rho a^3 \to 0$, where $\rho = (N+M)/|\Lambda|$ and a is the scattering length of the potential. The latter can be conveniently defined in terms of the solution to the zero energy scattering equation

$$-\Delta_x \varphi(x) + \frac{U}{2}\delta_{x,0}\varphi(x) = 0 \tag{1.4}$$

subject to the boundary condition $\lim_{|x|\to\infty}\varphi(x) = 1$. The solution is

$$\varphi(x) = 1 - 4\pi\frac{a}{r_0}\int_{|k_i|\leq \pi r_0^{-1}} \frac{d^3k}{(2\pi r_0^{-1})^3}\,\frac{e^{ikx}}{2\sum_{i=1}^3(1-\cos k_i r_0)} \tag{1.5}$$

where the coefficient a has the interpretation of scattering length and is given by

$$8\pi a = r_0\,\frac{U r_0^2}{U r_0^2\gamma + 1}\,, \qquad \gamma = \frac{1}{2}\int_{|k_i|\leq\pi}\frac{d^3k}{(2\pi)^3}\,\frac{1}{2\sum_{i=1}^3(1-\cos k_i)}\,. \tag{1.6}$$

Note that $\lim_{|x|\to\infty}(1-\varphi(x))|x| = a$ (this means that at large distances $\varphi(x)$ looks very much like the scattering solution in the continuum, i.e. $\varphi(x) \simeq 1 - a/|x|$ at large distances) and that $8\pi a \leq U r_0^3$ (this is the analogue of the inequality of Spruch and Rosenberg [SR] in the lattice

case). Another important remark is that, given any simply connected domain Ω containing the origin, the "flux" of the discrete derivative of $\varphi(x)$ across the boundary of Ω is independent of Ω and equal to $4\pi a$:

$$\sum_{<x,x'>}^{(\partial\Omega)} (\varphi(x') - \varphi(x)) = 4\pi a \tag{1.7}$$

where $\sum_{<x,x'>}^{(\partial\Omega)}$ is the sum over the bonds connecting nearest neighbor sites with $x \in \Omega$ and $x' \in \Omega^c$. This simply follows by the remark that $\Delta\varphi(x) = 0$, $\forall x \neq 0$, and by discrete "integration by parts".

B. Main results

We are now ready to state our main result.

Theorem 1. *Fix $\rho_\uparrow = N/|\Lambda|$, $\rho_\downarrow = M/|\Lambda|$ and $\rho = \rho_\uparrow + \rho_\downarrow$, and let $E_0(N, M, \Lambda)$ denote the ground state energy of H with the appropriate antisymmetry in each of the N, M coordinate variables. Then, for small ρa^3,*

$$\lim_{|\Lambda|\to\infty} \frac{1}{|\Lambda|} E_0(N, M, \Lambda) \leq e_0(\rho_\uparrow, \rho_\downarrow) + 8\pi a \rho_\uparrow \rho_\downarrow + a\rho^2 \varepsilon(\rho a^3), \tag{1.8}$$

where $e_0(\rho_\uparrow, \rho_\downarrow)$ is the specific ground state energy of the free Fermi gas on the lattice, i.e., of (1.3) with $U = 0$, and $0 \leq \varepsilon(\rho a^3) \leq \text{const}\,(\rho^{1/3}a)^{2/9}$.

Remarks.
1) The theorem is valid for any repulsion strength $U \geq 0$, including the limiting case $U = +\infty$ of infinite repulsion.
2) If $\rho r_0^3 \ll 1$, the specific ground state energy of the free Fermi gas on the lattice can be written as

$$e_0(\rho_\uparrow, \rho_\downarrow) = \frac{3}{5} \left(6\pi^2\right)^{2/3} (\rho_\uparrow^{5/3} + \rho_\downarrow^{5/3}) + \text{const } r_0^2 \rho^{7/3}$$

Then, as long as $a/r_0 \gg \sqrt{\rho^{1/3}a}$, in the r.h.s. of (1.8) we can replace $e_0(\rho_\uparrow, \rho_\downarrow)$ by $\frac{3}{5}\left(6\pi^2\right)^{2/3} (\rho_\uparrow^{5/3} + \rho_\downarrow^{5/3})$ and still have an error term that is much smaller than $\rho^2 a$. In this case the upper bound (1.8) looks precisely the same as (1.1).
3) It would be nice to establish that the r.h.s. of (1.8) is the correct low density behavior of the ground state energy of the 3D Hubbard model. In order to prove this we should provide a lower bound with the same asymptotic behavior as the r.h.s. of (1.8). The natural idea would be to proceed as in the continuum case [LSS], that is by exploiting Dyson's idea of replacing the "hard" interaction potential by a "soft" one, at the expense of using up some kinetic energy. Of course, in order to get the correct 0–th order contribution in the lower bound, we need to use at least part of the kinetic energy to "fill the Fermi sea": so technically one of the main steps in the proof of the lower bound in [LSS] is the proof of a "Dyson Lemma" in presence of an infrared cutoff, allowing for a replacement of the hard interaction by a soft one, at the expense only of the high momentum part of the kinetic energy. We would expect that this result is actually independent of the presence or absence of an underlying lattice structure: however the proof of the "Dyson Lemma" with infrared cutoff in [LSS] uses in a crucial way rotational invariance of the problem and it is an open problem to adapt it to the lattice case.

The result of the Theorem above, combined with the remark that the first term in the r.h.s. of (1.8) provides an obvious lower bound to the ground state energy, implies that $|E_0(N, M, \Lambda) - E_0^{(U=0)}(N, M, \Lambda)| \leq \text{const}\,|\Lambda| a \rho^2$ and this in turns implies that, if we fix the total density ρ and minimize the energy over the possible choices of $\rho_{\uparrow,\downarrow}$, we find that at low density the absolute ground state satisfies $|\rho_\uparrow - \rho_\downarrow| \leq \text{const}\,\rho\sqrt{\rho^{1/3}a}$ This implies that the

total spin S of the ground state satisfies the following.

Corollary 1. *Let S be the total spin in the absolute ground state of model (1.3) and let $S_{max} = (N+M)/2$. Then in the low density limit*

$$\lim_{|\Lambda|\to\infty} S/S_{max} \leq \text{const}\,\sqrt{\rho^{1/3}a} \tag{1.9}$$

where the thermodynamic limit is taken keeping the total density $\rho = (N+M)/|\Lambda|$ fixed.

Remark. It is natural to ask whether there exists some number $\rho_c > 0$ such that $\lim_{|\Lambda|\to\infty} S/S_{max} = 0$ for all $\rho < \rho_c$ (see Problem 4 in [Li]). Note that Corollary 1 does not exclude this possibility. Note also that proving or disproving this possibility requires necessarily some non perturbative argument: any approximate computation of the ground state energy can only improve the error term in the r.h.s. of (1.9) but will never establish the exact value of S/S_{max}.

II. THE UPPER BOUND

In this section we shall assume $a/r_0 > \delta^{-1}(\rho^{1/3}a)^{2/9}$, with δ a constant to be chosen below. In this case it is enough to prove the upper bound (1.8) with $e_0(\rho_\uparrow, \rho_\downarrow)$ replaced by $\frac{3}{5}\left(6\pi^2\right)^{2/3}(\rho_\uparrow^{5/3} + \rho_\downarrow^{5/3})$, see Remark (2) after the statement of the Theorem above. The weak coupling regime $a/r_0 \leq \delta^{-1}(\rho^{1/3}a)^{2/9}$ is much simpler and will be treated in Appendix B.

It will be convenient to localize the particles into small boxes with Dirichlet boundary conditions. The number of particles in each box will be large for small ρ, but finite and independent of the size of the large container Λ. Let the side length of the small boxes be ℓ. We then want to put $n = \rho_\uparrow \ell^3$ spin-up particles into each box, and likewise $m = \rho_\downarrow \ell^3$ spin-down particles (here $\rho_\uparrow = N|\Lambda|^{-1}$ and $\rho_\downarrow = M|\Lambda|^{-1}$). Since $\rho_{\uparrow,\downarrow}\ell^3$ need not be an integer, however, we will choose

$$n = \rho_\uparrow \ell^3 + \varepsilon_\uparrow \quad \text{and} \quad m = \rho_\downarrow \ell^3 + \varepsilon_\downarrow, \tag{2.1}$$

with $0 \leq \varepsilon_{\uparrow,\downarrow} < 1$ chosen such that n and m are integers. We then really have too many particles, but this is legitimate for an upper bound, since the energy is certainly increasing with particle number.

So, if $E_0(N, M, \Lambda)$ is the ground state energy of (1.3) in the box Ω, we have

$$\lim_{|\Lambda|\to\infty} \frac{1}{|\Lambda|} E_0(N, M, \Lambda) \leq \frac{1}{\ell^3} E_0(n, m, \Lambda_\ell), \tag{2.2}$$

where Λ_ℓ is the cubic box of side ℓ. Here we used that the interaction potential is zero range, so that different boxes of side ℓ are exactly decoupled. Note that actually the bound (2.2) is not only valid in the thermodynamic limit, but also for all finite cubic boxes Λ with side divisible by ℓ.

We will now derive an upper bound on the ground state energy of n spin-up and m spin-down particles in a cubic box of side length ℓ, for general n, m and ℓ. We take as a trial state the function

$$\Psi(X, Y) = D_n(X) D_m(Y) G_n(X) G_m(Y) F(X, Y), \tag{2.3}$$

where $D_n(X)$ denotes the Slater determinant of the first n eigenfunctions of the Laplacian in a cubic box of side length ℓ, with Dirichlet boundary conditions; note that, if $\phi_\alpha(x)$ are the eigenfunctions of the single-particle Laplacian in a cubic box of side length ℓ, we choose their normalization in such a way that $\sum_x r_0^3 \phi_\alpha^*(x)\phi_\beta(x) = \delta_{\alpha,\beta}$. Moreover,

$$G_n(X) = \prod_{1\leq i<j\leq n} g(x_i - x_j), \tag{2.4}$$

with $0 \le g(x) \le 1$, having the property that $g(x) = 0$ for $|x| \le s$ and $g(x) = 1$ for $|x| \ge 2s$, for some s to be chosen later. We can assume that for any pair of nearest neighbor points x and x' we have $|g(x') - g(x)| \le \mathrm{const}\, r_0 s^{-1}$ for some constant independent of s. Finally,

$$F(X,Y) = \prod_{i=1}^{n}\prod_{j=1}^{m} f(x_i - y_j), \tag{2.5}$$

where, given a simply connected domain $\Omega \subset \mathbb{Z}^3$ containing the origin, $f(x) = 1$ if $x \notin \Omega$. Inside Ω we choose $f(x)$ to be the solution to the zero-energy scattering equation with boundary conditions $f(x) = \varphi(x)/\langle\varphi\rangle_{\partial\Omega}$ on the boundary $\partial\Omega$ of the domain (here $\varphi(x)$ is given by (1.5), $\partial\Omega = \{x \in \Omega \,:\, \mathrm{dist}(x, \Omega^c) = 1\}$ and $\langle\varphi\rangle_{\partial\Omega} = |\partial\Omega|^{-1}\sum_{x\in\partial\Omega}\varphi(x)$). We shall make the following explicit choice for the domain: $\Omega = B_R \cap \mathbb{Z}^3$, where $B_R = \{x \in \mathbb{R}^3 \,:\, \varphi(x) \le 1 - a/R\}$. Note that, if $R \gg r_0$, B_R is approximately a ball of radius R. Moreover $\langle\varphi\rangle_{\partial\Omega} = 1 - a/R + O(ar_0/R^2)$ and, for any $x \in \partial\Omega$, $\varphi(x) = \langle\varphi\rangle_{\partial\Omega} + O(ar_0/R^2)$. We assume $\delta^{-1} r_0 < R \le s/5$, with δ the same constant as in the condition $a/r_0 > \delta^{-1}(\rho^{1/3}a)^{2/9}$ (to be chosen below).

By the variational principle,

$$E_0(n, m, \Lambda_\ell) \le \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}, \tag{2.6}$$

with

$$\langle\Psi|H|\Psi\rangle = \langle\Psi| - \Delta_X|\Psi\rangle + \langle\Psi| - \Delta_Y|\Psi\rangle + U\langle\Psi|v_{XY}|\Psi\rangle.$$

(here, for any operator $\hat{A}$, $\langle\Psi|\hat{A}|\Psi\rangle$ is defined as $\langle\Psi|\hat{A}|\Psi\rangle = \sum_{X,Y} r_0^{3(n+m)}\Psi(X,Y)\,\hat{A}\,\Psi(X,Y)$ – note the presence of the factor $r_0^{3(n+m)}$). We first evaluate $\langle\Psi| - \Delta_X|\Psi\rangle$. By definition it is equal to

$$\begin{aligned} &\frac{1}{r_0^2}\sum_{i=1}^{n}\sum_{X,Y} r_0^{3(n+m)} D_m(Y)^2 G_m(Y)^2 D_n(X) G_n(X) F(X,Y)\,\cdot \\ &\qquad \cdot \sum_{x_i' : |x_i' - x_i| = r_0} \Big[D_n(X)G_n(X)F(X,Y) - D_n(X_i')G_n(X_i')F(X_i', Y)\Big] \end{aligned} \tag{2.7}$$

where, if $X = \{x_1, \ldots, x_i, \ldots, x_{n_1}\}$, X_i' is given by $X_i' = \{x_1, \ldots, x_i', \ldots, x_{n_1}\}$. The r.h.s. of this equation can be written as

$$\begin{aligned} &\sum_{X,Y} r_0^{3(n+m)} D_m(Y)^2 G_m(Y)^2 G_n(X)^2 F(X,Y)^2 D_n(X)(-\Delta_X) D_n(X) \\ &+ \frac{1}{r_0^2}\sum_{i=1}^{n}\sum_{X,Y} r_0^{3(n+m)} \sum_{x_i' : |x_i' - x_i| = r_0} D_m(Y)^2 G_m(Y)^2 D_n(X) D_n(X_i')\,\cdot \\ &\qquad \cdot G_n(X)F(X,Y)\Big[G_n(X)F(X,Y) - G_n(X_i')F(X_i', Y)\Big] \end{aligned} \tag{2.8}$$

The first line is simply $E^D(n,\ell)\langle\Psi|\Psi\rangle$, where $E^D(n,\ell)$ is the sum of the lowest n eigenvalues of the Dirichlet Laplacian in the box of side ℓ (note that these eigenvalues are equal to $2r_0^{-2}\sum_{i=1}^{3}(1 - \cos k_i r_0)$, with k_i positive integer multiples of π/ℓ). An explicit computation shows that

$$E^{\mathrm{D}}(n,\ell) \le \frac{3}{5}(6\pi^2)^{2/3}\frac{n^{5/3}}{\ell^2}\Big(1 + \mathrm{const}\, n^{-1/3} + \mathrm{const}\, n^{2/3}(r_0/\ell)^2\Big) \tag{2.9}$$

The second line, if we symmetrize over X, X_i', can be rewritten as

$$\begin{aligned} &\frac{1}{r_0^2}\sum_{i=1}^{n}\sum_{X\setminus x_i, Y}\sum_{<x_i, x_i'>} r_0^{3(n+m)} D_m(Y)^2 G_m(Y)^2 D_n(X) D_n(X_i')\,\cdot \\ &\qquad \cdot \Big[G_n(X)F(X,Y) - G_n(X_i')F(X_i', Y)\Big]^2 \end{aligned} \tag{2.10}$$

where $\sum_{<x_i,x_i'>}$ is the sum over the nearest neighbor bonds in Λ_ℓ. By Cauchy-Schwarz, we can bound the last expression from above by

$$\frac{1}{r_0^2}\sum_{i=1}^{n}\sum_{X\setminus x_i,Y}\sum_{<x_i,x_i'>} r_0^{3(n+m)}D_m(Y)^2G_m(Y)^2D_n(X)^2\cdot \\ \cdot\Big[G_n(X)F(X,Y)-G_n(X_i')F(X_i',Y)\Big]^2 \tag{2.11}$$

We now use the Schwarz inequality to deduce (for some $\varepsilon>0$ to be chosen later)

$$\begin{aligned}&\Big[G_n(X)F(X,Y)-G_n(X_i')F(X_i',Y)\Big]^2\\ &\le(1+\varepsilon)G_n(X_i')^2\Big[F(X,Y)-F(X_i',Y)\Big]^2\\ &+(1+\varepsilon^{-1})F(X,Y)^2\Big[G_n(X)-G_n(X_i')\Big]^2\end{aligned} \tag{2.12}$$

Proceeding in the same way for the kinetic energy of the Y-particles, we thus get the upper bound

$$\langle\Psi|H|\Psi\rangle\le\big[E^{\rm D}(n,\ell)+E^{\rm D}(m,\ell)\big]\langle\Psi|\Psi\rangle+(1+\varepsilon)I_2+\big(1+\varepsilon^{-1}\big)\,I_3, \tag{2.13}$$

with:

$$\begin{aligned}I_2=\sum_{X,Y}r_0^{3(n+m)}D_n(X)^2D_m(Y)^2\ \cdot&\\ \cdot\Bigg\{G_m(Y)^2\frac{1}{2}\sum_{i=1}^{n}\sum_{x_i':|x_i'-x_i|=r_0}&G_n(X_i')^2\Big[\frac{F(X_i',Y)-F(X,Y)}{r_0}\Big]^2\\ +G_n(X)^2\frac{1}{2}\sum_{j=1}^{m}\sum_{y_j':|y_j'-y_j|=r_0}&G_m(Y_j')^2\Big[\frac{F(X,Y_j')-F(X,Y)}{r_0}\Big]^2\\ +UG_n(X)^2G_m(Y)^2v_{XY}F(X,Y)^2\Bigg\}&\end{aligned} \tag{2.14}$$

and

$$I_3=\sum_{X,Y}r_0^{3(n+m)}D_m(Y)^2D_n(X)^2F(X,Y)^2\cdot \\ \cdot\Big\{G_m(Y)^2|\nabla_XG(X)|^2+G_n(X)^2|\nabla_YG(Y)|^2\Big\} \tag{2.15}$$

where $|\nabla_XG(X)|^2=\sum_{i=1}^n|\nabla_iG(X)|^2$ and $|\nabla_iG(X)|^2=\frac{1}{2}\sum_{\omega=\pm}|\nabla_i^\omega G(X)|^2$. Moreover, for any function $g(x)$, the ω-gradient of g is defined as $\nabla^\omega g(x)=\sum_{\ell=1}^3\omega\hat{e}_\ell\big[g(x+\omega r_0\hat{e}_\ell)-g(x)\big]$ with $\hat{e}_\ell$ the coordinate versor in the ℓ-th direction. A similar definition is valid for $|\nabla_YG(Y)|^2$. The positivity of Uv_{XY} has been used here. Note that $E^{\rm D}(n,\ell)$ and $E^{\rm D}(m,\ell)$ can be bounded as in (2.9). We shall now bound I_2 and I_3, when divided by $\langle\Psi|\Psi\rangle$, separately.

Let us first derive an upper bound on I_2. We are going to need the following lemma [LSS].

Lemma 1. *Let $D_n(X)$ denote a Slater determinant of n linearly independent functions $\phi_\alpha(x)$. For a given function $h(x)$ of one variable, let $\Phi(X)$ be the function $\Phi(X)=D_n(X)\prod_{i=1}^n h(x_i)$, and let M denote the $n\times n$ matrix*

$$M_{\alpha\beta}=\sum_x r_0^3\phi_\alpha^*(x)\phi_\beta(x)|h(x)|^2\,. \tag{2.16}$$

Then the norm of Φ is given by $\langle\Phi|\Phi\rangle = \det M$. Moreover, for $1 \le k \le n$, the k-particle densities of Φ are given by

$$\binom{n}{k}\frac{1}{\langle\Phi|\Phi\rangle}\sum_{x_{k+1},\ldots,x_n} r_0^{3(n-k)}|\Phi(X)|^2 = \tag{2.17}$$
$$= \frac{1}{k!}\prod_{i=1}^{k}|h(x_i)|^2\big(x_1\wedge\cdots\wedge x_k\big|M^{-1}\otimes\cdots\otimes M^{-1}\big|x_1\wedge\cdots\wedge x_k\big),$$

where $|x)$ denotes the n-dimensional vector with components $\phi_\alpha(x)$, $1 \le \alpha \le n$, and $|x_1 \wedge \cdots \wedge x_k)$ stands for the Slater determinant $(k!)^{-1/2}\sum_\sigma(-1)^\sigma|x_{\sigma(1)})\otimes\cdots\otimes|x_{\sigma(k)})$, σ denoting permutations. Finally, if $\Phi'_i(X) = D_n(X)k(x_i)\prod_{j\neq i}h(x_j)$ for some function $k(x)$, then

$$\sum_{i=1}^{n}\langle\Phi'_i|\Phi'_i\rangle = \Big(\det M\Big)\Big(\mathrm{Tr}[KM^{-1}]\Big), \tag{2.18}$$

where $\mathrm{Tr}[\,\cdot\,]$ *denotes the trace, and K is the $n\times n$ matrix*

$$K_{\alpha\beta} = \sum_x r_0^3\phi_\alpha^*(x)\phi_\beta(x)|k(x)|^2\,. \tag{2.19}$$

Using $G_n(X'_i) \le 1$, we infer from this lemma that, for any fixed Y,

$$\begin{aligned}&\sum_X r_0^{3n}D_n(X)^2\Bigg\{\frac{1}{2}\sum_{i=1}^{n}\sum_{x'_i:|x'_i-x_i|=r_0}G_n(X'_i)^2\Big[\frac{F(X'_i,Y)-F(X,Y)}{r_0}\Big]^2\\&\qquad\qquad\qquad\qquad\qquad\qquad+\frac{U}{2}G_n(X)^2v_{XY}F(X,Y)^2\Bigg\}\\&\le\sum_X r_0^{3n}D_n(X)^2\Bigg\{|\nabla_XF(X,Y)|^2+\frac{U}{2}v_{XY}F(X,Y)^2\Bigg\}\\&=\mathrm{Tr}\{K_YM_Y^{-1}\}\sum_X r_0^{3n}D_n(X)^2F(X,Y)^2\end{aligned} \tag{2.20}$$

The $n\times n$ matrices K_Y and M_Y are given by (2.16) and (2.19), with $\phi_\alpha(x)$ being the lowest n Dirichlet eigenfunctions of $-\Delta$, and with $h(x) = \prod_j f(x-y_j)$ and

$$|k(x)|^2 = |\nabla h(x)|^2 + \frac{U}{2}\sum_j\delta_{x,y_j}\prod_j f(x-y_j)^2,$$

respectively (here $|\nabla h(x)|^2 = (2r_0^2)^{-1}\sum_{x':|x'-x|=r_0}|h(x)-h(x')|^2$, see definition after (2.15)).

Since K_Y is a positive definite matrix, we have the bound $\mathrm{Tr}K_YM_Y^{-1} \le \|M_Y^{-1}\|\mathrm{Tr}K_Y$, where $\|\cdot\|$ denotes the (spectral) matrix norm. To calculate $\mathrm{Tr}K_Y$, and to bound $\|M_Y^{-1}\|$, we can assume that all the y_j's are separated by at least a distance s, because the summand in (2.14) vanishes otherwise.

Since $s \ge 5R$ by assumption, we have in this case $|k(x)|^2 = \sum_{j=1}^n\xi(x-y_j)$ with

$$\xi(x-y) = |\nabla f(x-y)|^2 + \frac{U}{2}\delta_{x,y}f(x-y)^2\,. \tag{2.21}$$

Hence, if $\rho_n^D(x)$ denotes the one-particle density of $D_n(X)$, we have

$$\mathrm{Tr}K_Y = \sum_{j=1}^{m}\sum_x r_0^3\rho_n^D(x)\xi(x-y_j) \stackrel{def}{=} \sum_{j=1}^{m}\rho_n^D*\xi(y_j), \tag{2.22}$$

where $*$ denotes convolution. In order to bound $\|M_Y^{-1}\|$, we use the following:

Lemma 2. *Assume that* $|y_i - y_j| \geq s \geq 5R$ *for all* $i \neq j$. *Then if* r_0/R, n^{-1} *and* $n(r_0/\ell)^3$ *are sufficiently small*

$$\|1 - M_Y\| \leq \text{const}\left(\frac{aR^2}{s^3} + n^{2/3}\frac{s^2}{\ell^2}\right). \tag{2.23}$$

Proof. Let $q(x) = 1 - \prod_j f(x-y_j)^2 \geq 0$. Then, for any n-dimensional vector $|b)$ with components b_α,

$$\big(b\big|1 - M_Y\big|b\big) = \sum_x r_0^3 q(x)\Big|\sum_\alpha b_\alpha \phi_\alpha(x)\Big|^2.$$

Hence, the question about the largest eigenvalue of $1 - M_Y$ translates into the question of how large the average potential energy for the potential $q(x)$ can be for functions such as $\sum_\alpha b_\alpha\phi_\alpha(x)$ whose kinetic energy is bounded above by (const.) $n^{2/3}\ell^{-2}$, i.e., the Fermi energy for n particles (under the assumption that $n \gg 1$ and $nr_0^3 \ll \ell^3$).

Let Q_j denote the cube of side $s/2$ centered at y_j. Note that all these cubes are non-overlapping by assumption. Also, since $s \geq 5R$, $q(x) = 0$ if x is outside all the cubes (recall that by definition – see the lines following (2.5) – $f(x)$ is identically 1 outside a region B_R of radius $R\left[1 + O\big((r_0/R)^\kappa\big)\right]$, for some $\kappa > 0$). For a given function $\phi(x)$, let ϕ_j denote the average of $\phi(x)$ in the cube Q_j. Moreover, let $\eta(x) = \phi(x) - \phi_j$. By the Cauchy-Schwarz inequality $(a+b)^2 \leq 2(a^2+b^2)$, we get the bound

$$\sum_{x\in Q_j} q(x)|\phi(x)|^2 \leq 2\sum_{x\in Q_j} q(x)|\eta(x)|^2 + 2|\phi_j|^2\sum_{x\in Q_j} q(x). \tag{2.24}$$

Note that $|\phi_j|^2 \leq 8s^{-3}\sum_{x\in Q_j} r_0^3|\phi(x)|^2$, again by the Cauchy-Schwarz inequality. Moreover, since $s \geq R$,

$$\sum_{x\in Q_j} r_0^3 q(x) = \sum_{x\in B_R} r_0^3(1 - f(x)^2) \leq \text{const}\, aR^2.$$

To obtain the last inequality, we used that if $x \in B_R$ then $f(x) = \varphi(x)/\langle\varphi\rangle_{\partial\Omega} \geq \varphi(x)$, with $\varphi(x)$ defined in (1.5).

Note that $\eta(x)$ is a function whose average over the cube Q_j is zero. In other words, it is orthogonal to the constant function in Q_j. Hence, using the fact that $q(x) \leq 1$:

$$\begin{aligned}\sum_{x\in Q_j} r_0^3 q(x)|\eta(x)|^2 \quad &\leq \sum_{x\in Q_j} r_0^3|\eta(x)|^2 \\ &\leq \frac{1}{2(1-\cos(2\pi r_0 s^{-1}))}\sum_{\substack{x,x'\in Q_j\\ |x-x'|=r_0}} r_0^3|\eta(x)-\eta(x')|^2\,,\end{aligned} \tag{2.25}$$

where we used that $2r_0^{-2}(1-\cos(2\pi r_0 s^{-1}))$ is the second eigenvalue of the discrete Neumann Laplacian in the cube of side $s/2$ and mesh r_0. In this last expression we can replace $\eta(x)$ by $\phi(x)$, of course, since they only differ by a constant. Summing over all the cubes Q_j (and using that $q(x) = 0$ outside the cubes), we thus obtain that, for any function $\phi(x)$,

$$\sum_x r_0^3 q(x)|\phi(x)|^2 \ \leq \text{const}\left[\frac{aR^2}{s^3}\sum_x r_0^3|\phi(x)|^2 \ + s^2\sum_x r_0^3|\nabla\phi(x)|^2\right].$$

In the case in question, the kinetic energy of $\phi(x)$ is bounded by const $n^{2/3}\ell^{-2}$. This finishes the proof of the lemma. ■

Since $0 \leq M_Y \leq 1$ as a matrix, this lemma implies that

$$\|M_Y^{-1}\| = \frac{1}{1 - \|1 - M_Y\|} \leq A_n \equiv \frac{1}{1 - \text{const}\left[aR^2/s^3 + n^{2/3}(s/\ell)^2\right]}, \tag{2.26}$$

provided the denominator is positive. By inserting (2.22) and (2.26) into (2.20), we see that, for fixed Y with $|y_i - y_j| \geq s$ for all $i \neq j$,

$$\sum_X r_0^{3n} D_n(X)^2 \left\{ |\nabla_X F(X,Y)|^2 + \frac{U}{2} v_{XY} F(X,Y)^2 \right\}$$
$$\leq A_n \sum_{j=1}^n \rho_n^{\mathrm{D}} * \xi(y_j) \sum_X r_0^{3n} D_n(X)^2 F(X,Y)^2 \,. \tag{2.27}$$

To be able later to compare this expression (2.27) with $\langle \Psi | \Psi \rangle$, we want to put $G_n(X)^2$ back into the integrand. For this purpose we need the following lemma, which compares the integrals with and without the factor $G_n(X)^2$.

Lemma 3. *For any fixed Y, if n^{-1} and $n(r_0/\ell)^3$ are sufficiently small*

$$\sum_X \quad r_0^{3n} D_n(X)^2 F(X,Y)^2 G_n(X)^2$$
$$\geq \sum_X r_0^{3n} D_n(X)^2 F(X,Y)^2 \ \left(1 - \mathrm{const}\, n^{8/3} \|M_Y^{-1}\|^2 (s/\ell)^5\right) . \tag{2.28}$$

Proof Since $g(x) = 1$ for $|x| \geq 2s$, we have

$$G_n(X)^2 \geq 1 - \sum_{i<j}^n \theta(2s - |x_i - x_j|). \tag{2.29}$$

Here θ denotes the Heaviside step function, i.e., $\theta(t) = 1$ for $t \geq 0$ and $\theta(t) = 0$ for $t < 0$. To evaluate the sum involving the second term in (2.29), we need the two-particle density of the state $D_n(X)F(X,Y)$ for each fixed Y. By Lemma 1 above, and the fact that $f(x) \leq 1$, this density, when appropriately normalized, is bounded from above by $\|M_Y^{-1}\|^2 \rho_n^{\mathrm{D},(2)}(x,x')$, where $\rho_n^{\mathrm{D},(2)}(x,x')$ denotes the two-particle density of the determinantal state $D_n(X)$. In particular, by explicit computation one finds that, if $n \gg 1$ and $nr_0^3 \ll \ell^3$, this latter density satisfies the bound

$$\rho_n^{\mathrm{D},(2)}(x,x') \leq \mathrm{const}\, |x - x'|^2 (n/\ell^3)^{8/3} \tag{2.30}$$

for some constant independent of n and ℓ. Hence we arrive at (2.28). ■

Let

$$B_n = \left(1 - \mathrm{const}\, n^{8/3} A_n^2 (s/\ell)^5\right)^{-1},$$

assuming that the term in parenthesis is positive. Applying Lemma 3 to inequality (2.27), we arrive at

$$\sum_{XY} r_0^{3(n+m)} G_n(X)^2 D_n(X)^2 \left[|\nabla_X F(X,Y)|^2 + \frac{U}{2} v_{XY} F(X,Y)^2 \right] D_m(Y) G_m(Y)$$
$$\leq A_n B_n \sum_{j=1}^n \sum_{XY} r_0^{3(n+m)} \rho_n^{\mathrm{D}} * \xi(y_j) D_m(Y)^2 D_n(X)^2 F(X,Y)^2 G_m(Y)^2 G_n(X)^2 \,. \tag{2.31}$$

Now we cannot bound $\rho_n^{\mathrm{D}} * \xi(y)$ independently of y by simply using the supremum of $\rho_n^{\mathrm{D}}(x)$, since this number will be strictly bigger than n/ℓ^3, even in the thermodynamic limit. Instead, we repeat the above argument for the Y integration. We use $|G_m(Y)| \leq 1$, the Y-analogues of Lemma 1 and then Lemma 3 to put $G_m(Y)^2$ back in. Here, it is important to note that now the x_i's are separated by at least a distance $s \geq 5R$. In this way we obtain

$$\sum_{X,Y} r_0^{3(n+m)} G_n(X)^2 D_n(X)^2 \left[|\nabla_X F(X,Y)|^2 + \frac{U}{2} v_{XY} F(X,Y)^2 \right] D_m(Y) G_m(Y)$$
$$\leq A_n B_n B_m \sum_{XY} r_0^{3(n+m)} D_m(Y)^2 D_n(X)^2 F(X,Y)^2 G_m(Y)^2 G_n(X)^2 \,\mathrm{Tr} \widehat{K}_X M_X^{-1} \tag{2.32}$$

The matrix M_X is the same as before, with Y replaced by X (and n replaced by m, of course), and $\widehat{K}_X$ is the $m\times m$ matrix

$$(\widehat{K}_X)_{\alpha\beta} = \sum_y r_0^3 \phi_\alpha(y)^* \phi_\beta(y) \prod_i f(y-x_i)^2 \rho_n^{\rm D} * \xi(y)\,.$$

Using $|f(x)|\le 1$ and $\|M_X^{-1}\|\le A_m$, which follows from Lemma 2 and the fact that the x_i's are separated at least by a distance s, we get the bound

$$\mathrm{Tr}\widehat{K}_X M_X^{-1} \le A_m \mathrm{Tr}\widehat{K}_X \le A_m \sum_{x,y} r_0^6 \rho_n^{\rm D}(x)\rho_m^{\rm D}(y)\xi(x-y)\,. \tag{2.33}$$

A computation (see Appendix A) shows that

$$\sum_x r_0^3 \xi(x) \le 4\pi a (1+\mathrm{const}\, a/R)\,. \tag{2.34}$$

We then use this information to bound the last sum in (2.33), by using Schwarz's inequality:

$$\begin{aligned}
&\sum_{x,y} r_0^6 \rho_n^{\rm D}(x)\rho_m^{\rm D}(y)\xi(x-y)\\
&\quad\le \left(\sum_{x,y} r_0^6 \rho_n^{\rm D}(x)^2\xi(x-y)\right)^{1/2}\left(\sum_{x,y} r_0^6 \rho_m^{\rm D}(y)^2\xi(x-y)\right)^{1/2}\\
&\quad= \left(\sum_x r_0^3\rho_n^{\rm D}(x)^2\right)^{1/2}\left(\sum_y r_0^3\rho_m^{\rm D}(y)^2\right)^{1/2}\sum_x r_0^3\xi(x)\\
&\quad\le \left(\sum_x r_0^3\rho_n^{\rm D}(x)^2\right)^{1/2}\left(\sum_y r_0^3\rho_m^{\rm D}(y)^2\right)^{1/2} 4\pi a\,(1+\mathrm{const}\,\frac{a}{R}).
\end{aligned} \tag{2.35}$$

For the square of $\rho_n^{\rm D}(x)$, by an explicit computation we find

$$\sum_x r_0^3 \rho_n^{\rm D}(x)^2 \le \frac{n^2}{\ell^3}\Big(1+\mathrm{const}\, n^{-1/3} + \mathrm{const}\, n^{2/3}(r_0/\ell)^2\Big)\,. \tag{2.36}$$

The same holds with n replaced by m. Eq. (2.32) thus implies the upper bound

$$\begin{aligned}
&\sum_{XY} r_0^{3(n+m)} G_n(X)^2 D_n(X)^2 \left[|\nabla_X F(X,Y)|^2 + \frac{U}{2} v_{XY} F(X,Y)^2\right] D_m(Y) G_m(Y)\\
&\le \langle\Psi|\Psi\rangle \frac{4\pi a n m}{\ell^3} A_n A_m B_n B_m \cdot\\
&\quad\cdot\left[1+\mathrm{const}\,\left(\frac{a}{R}+n^{-1/3}+m^{-1/3}+(n+m)^{2/3}(r_0/\ell)^2\right)\right].
\end{aligned} \tag{2.37}$$

The same bound holds, of course, with X and Y interchanged. We therefore have the upper bound

$$\begin{aligned}
I_2 \le \langle\Psi|\Psi\rangle \frac{8\pi a n m}{\ell^3} A_n A_m B_n B_m \cdot&\\
\cdot\left[1+\mathrm{const}\,\left(\frac{a}{R}+n^{-1/3}+m^{-1/3}+(n+m)^{2/3}(r_0/\ell)^2\right)\right].&
\end{aligned} \tag{2.38}$$

It remains to bound the term I_3. Using $|g(x)|\le 1$ we have that

$$\begin{aligned}
|\nabla_X G_n(X)|^2 \le \frac{1}{2}\sum_{\omega=\pm}\Bigg[&\sum_{i=1}^n \sum_{j,\,j\ne i} |\nabla^\omega g(x_i-x_j)|^2\\
&+\sum_{i=1}^n \sum_{j,\,j\ne i}\sum_{k,\,k\ne i,j} |\nabla^\omega g(x_i-x_j)\cdot\nabla^\omega g(x_i-x_k)|\Bigg],
\end{aligned} \tag{2.39}$$

where the ω-gradient ∇^ω was defined after (2.15). Now, by Lemma 1, the appropriately normalized k-particle densities of $D_n(X)F(X,Y)$ are bounded above by $\|M_Y^{-1}\|^k \rho_n^{\mathrm{D},(k)}$, where $\rho_n^{\mathrm{D},(k)}$ denotes the k-particle density of $D_n(X)$. In particular, $\rho_n^{\mathrm{D},(2)}$ satisfies the bound (2.30), and $\rho_n^{\mathrm{D},(3)}$ satisfies

$$\rho_n^{\mathrm{D},(3)}(x,x',x'') \leq \mathrm{const}\,(n/\ell^3)^3$$

for some constant independent of n and ℓ. Remember that, by the definition of g (see lines following (2.4)), if x and x' are two neighbor points, $g(x')-g(x)$ is zero for $|x|>2s$ and otherwise $|g(x')-g(x)| \leq \mathrm{const}\, r_0 s^{-1}$. Using this, we obtain from (2.39), for any fixed Y,

$$\begin{aligned}
&\sum_X r_0^{3n} D_n(X)^2 F(X,Y)^2 |\nabla_X G_n(X)|^2 \qquad (2.40)\\
&\leq \mathrm{const}\,\frac{n^2}{\ell^3} s \left(\|M_Y^{-1}\|^2 n^{2/3}(s/\ell)^2 + \|M_Y^{-1}\|^3 n (s/\ell)^3\right) \sum_X r_0^{3n} D_n(X)^2 F(X,Y)^2 \,.
\end{aligned}$$

Finally, to get a bound on I_3, we proceed as above, using (2.26) (and the fact that the y_j's are separated by a distance s) and Lemma 3 to put $G_n(X)^2$ back into the integral. Note, however, that it is enough to bound A_n and B_n by constants in this term. Assuming that $n(s/\ell)^3$ is small, the second term in the parenthesis in (2.40) is negligible compared to the first term. The same bound applies to the case where X and Y are interchanged, and hence we obtain

$$I_3 \leq \langle\Psi|\Psi\rangle\,\mathrm{const}\left(n^{8/3}+m^{8/3}\right)\frac{s^3}{\ell^5}. \qquad (2.41)$$

Collecting all the error terms obtained in Eqs. (2.9), (2.38) and (2.41) and inserting them into (2.6) and (2.13), we obtain

$$\begin{aligned}
&E_0(n,m,\Lambda_\ell) \leq \\
&\quad \leq \frac{3}{5}(6\pi^2)^{2/3}\frac{n^{5/3}+m^{5/3}}{\ell^2}\left(1+Cn^{-1/3}+Cm^{-1/3}+C(n+m)^{2/3}(r_0/\ell)^2\right)\\
&\quad +8\pi a\frac{nm}{\ell^3}\left(1+\varepsilon+C\left[\frac{aR^2}{s^3}+(n+m)^{2/3}(s/\ell)^2\right.\right.\\
&\quad \left.\left.+\frac{a}{R}+\frac{1}{n^{1/3}}+\frac{1}{m^{1/3}}+(n+m)^{8/3}(s/\ell)^5\right]\right) \qquad (2.42)\\
&\quad +\frac{Cs}{\varepsilon}\frac{(n+m)^2}{\ell^3}\left[(n+m)^{2/3}(s/\ell)^2\right]
\end{aligned}$$

for some constant $C>0$. In Ineq. (2.42) we have assumed smallness of all the error terms, i.e., that the terms in square brackets are small. This condition will be fulfilled, at low density, with our choice of R, s, n, m and ℓ below.

The optimal choice of ε in (2.42) is given by $\varepsilon^2 = \mathrm{const}\,(n+m)^{8/3}s^3/(\ell^2 anm)$. Inserting this value for ε we infer from (2.42)

$$\begin{aligned}
&E_0(n,m,\Lambda_\ell) \leq \\
&\quad \leq \frac{3}{5}(6\pi^2)^{2/3}\frac{n^{5/3}+m^{5/3}}{\ell^2}\left(1+Cn^{-1/3}+Cm^{-1/3}+C(n+m)^{2/3}(r_0/\ell)^2\right)\\
&\quad +8\pi a\frac{nm}{\ell^3}\left(1+C\left[\frac{aR^2}{s^3}+(n+m)^{2/3}(s/\ell)^2\right.\right.\\
&\quad \left.\left.+\frac{a}{R}+\frac{1}{n^{1/3}}+\frac{1}{m^{1/3}}+(n+m)^{8/3}(s/\ell)^5\right]\right) \qquad (2.43)\\
&\quad +C(n+m)^{7/3}\frac{s^{3/2}a^{1/2}}{\ell^4}.
\end{aligned}$$

Eq. (2.44) is our final bound on the energy $E_0(n,m,\ell)$. To apply this result in (2.2) we have to insert the values (2.1) for n and m. Recall that $|n-\rho_\uparrow\ell^3|\leq 1$ and $|m-\rho_\downarrow\ell^3|\leq 1$. We are

then still free to choose R, s and ℓ. We choose

$$R = a\big(a\rho^{1/3}\big)^{-2/9}\ ,\ s = 6R\ ,\ \ell = \rho^{-1/3}\big(a\rho^{1/3}\big)^{-11/9}.$$

Note that with these choices the condition $a/r_0 > \delta^{-1}(\rho^{1/3}a)^{2/9}$ implies $r_0/R < \delta$. We choose δ to be so small that Lemma 2 is valid. Inserting these values into (2.44) we thus obtain, for small ρ,

$$\frac{1}{\ell^3}E_0(n,m,\Lambda_\ell) \le \frac{3}{5}(6\pi^2)^{2/3}\big[\rho_\uparrow^{5/3}+\rho_\downarrow^{5/3}\big] + 8\pi a\rho_\uparrow\rho_\downarrow + \mathrm{const}\, a\rho^2\big(a\rho^{1/3}\big)^{2/9}.$$

In combination with Eq. (2.2), this finishes the proof of the upper bound in the case $a/r_0 \ge \delta^{-1}(\rho^{1/3}a)^{2/9}$. The opposite case (that is much simpler) is treated in Appendix B.

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APPENDIX A: PROOF OF (2.34)

In this Appendix we want to show that if $\xi(x)$ is defined by (2.21) then $\sum_x r_0^3\xi(x) \le 4\pi a(1+\mathrm{const}\, a/R)$. Note that "integrating by parts" we can rewrite the summation as:

$$\sum_x r_0^3\xi(x) = \sum_x r_0^3 f(x)(-\Delta_x)f(x) + \frac{U}{2}f(0)^2 \tag{A.1}$$

Note also that, by definition, if $x\in\Omega$ then $f(x)$ coincides with $\varphi(x)/\langle\varphi\rangle_{\partial\Omega}$, while if $x\notin\Omega$ then $f(x)=1$. Then, by the definition of $\varphi(x)$, we see that in the summation in (A.1) all terms with x "well inside" Ω (i.e. with x such that $\mathrm{dist}(x,\Omega^c)\ge 2r_0$) cancel out with $\frac{U}{2}f(0)^2$, and all terms with x "well outside" Ω (i.e. with x such that $\mathrm{dist}(x,\Omega)\ge 2r_0$)) are identically zero. So we are left with a boundary term, that is a summation over the x's at a distance r_0 from Ω or from Ω^c. Let us recall that $\partial\Omega = \{x\in\Omega : \mathrm{dist}(x,\Omega^c)=r_0\}$ and let us define $\partial\Omega^c = \{x\in\Omega^c : \mathrm{dist}(x,\Omega)=r_0\}$. The r.h.s. of (A.1) can be rewritten as

$$\begin{aligned}&\sum_{x\in\partial\Omega} r_0^3 f(x)(-\Delta)f(x) + \sum_{x'\in\partial\Omega^c} r_0^3 f(x')(-\Delta)f(x') \\ &= \sum_{x\in\partial\Omega} r_0\frac{\varphi(x)}{\langle\varphi\rangle_{\partial\Omega}}\sum_{x'\in\partial\Omega^c}^{(x)}\left[\frac{\varphi(x')}{\langle\varphi\rangle_{\partial\Omega}}-1\right] + \sum_{x'\in\partial\Omega^c} r_0\sum_{x\in\partial\Omega}^{(x')}\left[1-\frac{\varphi(x)}{\langle\varphi\rangle_{\partial\Omega}}\right]\end{aligned} \tag{A.2}$$

where $\sum_{x'\in\partial\Omega^c}^{(x)}$ is the sum over the points $x'\in\partial\Omega^c$ at a distance r_0 from x (and similarly for $\sum_{x\in\partial\Omega}^{(x')}$). The second line in (A.2) can still be rewritten as

$$\sum_{x\in\partial\Omega} r_0\left[\frac{\varphi(x)}{\langle\varphi\rangle_{\partial\Omega}}-1\right]\sum_{x'\in\partial\Omega^c}^{(x)}\left[\frac{\varphi(x')}{\langle\varphi\rangle_{\partial\Omega}}-1\right] + \frac{1}{\langle\varphi\rangle_{\partial\Omega}}\sum_{<x,x'>}^{*} r_0\left[\varphi(x')-\varphi(x)\right] \tag{A.3}$$

where $\sum_{<x,x'>}^{*}$ is the sum over the nearest neighbor pairs $<x,x'>$ with $x\in\partial\Omega$ and $x'\in\partial\Omega^c$. Recall that, if $R\gg r_0$, then for any $x\in\partial\Omega$ and any $x'\in\partial\Omega^c$ we have $\varphi(x),\varphi(x') = \langle\varphi\rangle_{\partial\Omega}+O(ar_0/R^2)$. Then the first term in (A.3) can be bounded above by a constant times $(R^2/r_0^2)r_0(ar_0/R^2)^2 = a(ar_0/R^2) < a(a/R)$. Moreover, note that the second term in (A.3) is proportional to the (discrete) flux of the discrete derivative of φ across the "surface" of Ω and the latter is *equal* to $4\pi a$, see (1.7). As a conclusion, the second term in (A.3) is equal to $4\pi a/\langle\varphi\rangle_{\partial\Omega}$. Using that $\langle\varphi\rangle_{\partial\Omega} = 1-a/R+O(ar_0/R^2)$, see lines following Eq. (2.5), (2.34) is proven.

APPENDIX B: THE WEAK COUPLING REGIME

In this Appendix we prove the main Theorem in the case that $a/r_0 \leq \delta^{-1}(\rho^{1/3}a)^{2/9}$. In this case we do not localize particles and we simply choose as trial function the ground state of the free Fermi gas: $\Psi(X,Y) = D_N(X)D_M(Y)$, where $D_N(X)$ denotes the Slater determinant of the first N eigenfunctions of the Laplacian in the cubic box Λ with (say) periodic boundary conditions (a similar definition is valid for $D_M(Y)$). We assume that $D_N(X)$ and $D_M(Y)$ are normalized in such a way that $\langle\Psi|\Psi\rangle = \sum_{X,Y} r_0^{3(N+M)}|D_N(X)|^2|D_M(Y)|^2 = 1$. By the variational principle $E_0(N,M,\Lambda) \leq \langle\Psi|H|\Psi\rangle = E_0^{(U=0)}(N,M,\Lambda) + U\sum_{i=1}^N \sum_{j=1^M} \langle\Psi|v_{X,Y}|\Psi\rangle$. Since the specific energy corresponding to the term $E_0(N,M,\Lambda)|_{U=0}$ is by definition $e_0(\rho_\uparrow,\rho_\downarrow)$, we are left with bounding

$$\sum_Y r_0^{3M}|D_M(Y)|^2 \sum_{i=1}^N \sum_X r_0^{3N}|D_N(X)|^2 \sum_{j=1}^M \delta_{x_i,y_j} \tag{B.1}$$

An application of Lemma 1 shows that this expression is equal to $\sum_x r_0^6 \rho_N(x)\rho_M(x)$, where ρ_N is the 1-particle density of $D_N(X)$ and ρ_M is the 1-particle density of $D_N(Y)$. In our case $\rho_N(x) \equiv \rho_\uparrow$ and $\rho_M(x) \equiv \rho_\downarrow$. Then we get $U\sum_{i=1}^N \sum_{j=1^M} \langle\Psi|v_{X,Y}|\Psi\rangle = |\Lambda|Ur_0^3\rho_\uparrow\rho_\downarrow$. By (1.6) we have that $Ur_0^3 = 8\pi a(1+\gamma U r_0^2)$. As a conclusion:

$$\lim_{|\Lambda|\to\infty} \frac{1}{|\Lambda|} E_0(N,M,\Lambda) \leq e_0(\rho_\uparrow,\rho_\downarrow) + 8\pi a\rho_\uparrow\rho_\downarrow(1+\gamma U r_0^2) \tag{B.2}$$

Since $Ur_0^2 = 8\pi a/r_0(1 + \mathrm{const}\, a/r_0)$, we have that $\gamma U r_0^2 \leq \mathrm{const}\,(\rho^{1/3}a)^{2/9}$ and the proof is concluded.

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